

Some Exact Results for the Schrödinger Wave Equation with a Time Dependent Potential

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Abstract

The time dependent Schrödinger equation with a time dependent delta function potential is solved exactly for many special cases. In all other cases the problem can be reduced to an integral equation of the Volterra type. It is shown that by knowing the wave function at the origin, one may derive the wave function everywhere. Thus, the problem is reduced from a PDE in two variables to an integral equation in one. These results are used to compare adiabatic versus sudden changes in the potential. It is shown that adiabatic changes in the potential lead to conservation of the normalization of the probability density.

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Introduction

Very few cases of the time dependent Schrödinger wave equation with a time dependent potential can be solved exactly. The cases that are known include the time dependent harmonic oscillator,[1-3] an example of an infinite potential well with a moving boundary,[4-6] and various other special cases. There remain, however, a large number of time dependent problems that, at least in principal, can be solved exactly.

One case that has been looked at over the years is the delta function potential. The author first investigated this problem in the mid 1980s [7] as an unpublished work. This was later included as part of a PhD thesis dissertation [8] but not published in a journal. In that work the Schrödinger wave equation with a strength that varies as a function of time was investigated. That work was more extensive than what we present here in that it also included the periodic time dependence and a delta function array with time dependence. In the time that has transpired since then, much (published) work has been done in relation to time evolution delta function potential problems. Most of that has focused on the time evolution/propagator derivation of the case of one or more delta functions with constant amplitude in time. In contrast, this work deals mainly with a potential with a strength that varies in time.

There are two types of time dependent problems that are commonly investigated. The problem that has received the most attention over the years is the simple scattering problem where one seeks what amounts to a steady state solution where the potential has a periodic dependence on time. In the case of the delta function potential, this problem was investigated where the strength varied sinusoidally in time[9]. Using Floquet formalism, they were able to derive a transmission coefficient as a function of driving frequency and amplitude. Other examples of scattering problems involving delta function

potentials also exist in the literature [10]. The actual solutions, however, are simple plane waves.

The other time dependent problem is where one starts with an initial state and allows that to evolve in time. These are the diffusive solutions to the Schrödinger wave equation. This and the closely related problem of finding the propagator have been investigated in some depth in relation to the one or more delta function potential [11-16]. Out of those cases cited only one of them involves a potential with true time dependence [13] and that is the case of two delta functions that move apart from one another at constant velocity. There are two common approaches one may use. One method is using a path integral of the Feynman type and the other is using Laplace transforms. We use the latter though the two methods are closely related.

Formulation of the Problem

We would like to solve the Schrödinger equation with a time dependent potential,

$$\begin{aligned} -\psi_{xx} + 2c(t)\delta(x)\psi &= i\psi_t \\ \psi &\rightarrow 0, x \rightarrow \pm\infty \end{aligned} \quad (1)$$

By integrating Equation 1 over the discontinuity at $x=0$, we find that the problem reduces to,

$$\begin{aligned} -\psi_{xx} &= i\psi_t \\ \psi_x(0^+, t) - \psi_x(0^-, t) &= 2c(t)\psi(0, t) \\ \psi &\rightarrow 0, x \rightarrow \pm\infty \end{aligned} \quad (2)$$

This is just the case of zero potential with an additional time dependent boundary condition. If we restrict ourselves to $t>0$, we may take the Laplace transform of Equation

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$$\begin{aligned} -\bar{\psi}_{xx} &= is\bar{\psi} - i\psi(x, 0) \\ \bar{\psi}_x(0^+, s) - \bar{\psi}_x(0^-, s) &= 2L[c(t)\psi(0, t)] \end{aligned} \quad (3)$$

We now solve Equation 3. However, we must consider the homogeneous solution in order to satisfy the cusp condition at the origin. The solution is

$$\bar{\psi}(x,s) = a(s) \exp(i\sqrt{is}|x|) + \frac{1}{2\sqrt{is}} \int dx' \exp(i\sqrt{is}|x-x'|) \psi(x',0) \quad (4)$$

where $a(s)$ is an arbitrary function of s , yet to be determined. By applying the cusp condition at the origin to Equation 2.4 we find

$$\begin{aligned} \bar{\psi}_x(0^+,s) - \bar{\psi}_x(0^-,s) &= 2i\sqrt{is}a(s) = 2L[c(t)\psi(0,t)] \\ \Rightarrow a(s) &= \frac{L[c(t)\psi(0,t)]}{i\sqrt{is}} \end{aligned} \quad (5)$$

We now set $x=0$ in Equation 4 and use the results of Equation 5 to find

$$\bar{\psi}(0,s) = \frac{L[c(t)\psi(0,t)]}{i\sqrt{is}} + \frac{1}{2\sqrt{is}} \int_{-\infty}^{\infty} dx' \exp(i\sqrt{is}|x'|) \psi(x',0) \quad (6)$$

Using the convolution theorem for Laplace transforms [17], we invert Equation 6 to find

$$\psi(0,t) - \frac{1}{i\sqrt{i\pi}} \int_0^t dt' \frac{c(t')\psi(0,t')}{\sqrt{t-t'}} = \frac{1}{2\sqrt{i\pi t}} \int_{-\infty}^{\infty} dx' \exp\left(i \frac{(x')^2}{4t}\right) \psi(x',0) \quad (7)$$

Equation 7 is a Volterra integral equation that determines the wave function at the origin. Once the wave function at the origin is known, one may find the wave function everywhere by inverting Equation 4 which has the result

$$\psi(x,t) = \frac{1}{i\sqrt{i\pi}} \int_0^t dt' \frac{c(t')\psi(0,t')}{\sqrt{t-t'}} \exp\left(i \frac{x^2}{4(t-t')}\right) + \frac{1}{2\sqrt{i\pi t}} \int_{-\infty}^{\infty} dx' \exp\left(i \frac{(x-x')^2}{4t}\right) \psi(x',0) \quad (8)$$

Equations 7 and 8 completely determine the problem. As we can see knowing the wave function at the origin is equivalent to knowing the wave function everywhere.

Some Specific Cases

Derivation of the Propagator for Constant c and Jumps

In some situations it is advantageous to represent the solution in the form,

$$\psi(x,t) = \int_{-\infty}^{\infty} dx' G(x,x',t) \psi(x',0) \quad (9)$$

where G is the propagator. To find the propagator, we use Equations 5 and 6 to find,

$$a(s) = \frac{c \bar{\psi}(0,s)}{i\sqrt{is}} = -\frac{c}{2} \frac{1}{\sqrt{s}} \frac{1}{\sqrt{s} + \sqrt{ic}} \int_{-\infty}^{\infty} dx' \exp(i\sqrt{is}|x'|) \psi(x',0) \quad (10)$$

By Equations 4 and 10, we find,

$$\bar{G}(x,x',s) = -\frac{c}{2} \frac{\exp(i\sqrt{is}(|x| + |x'|))}{\sqrt{s}(\sqrt{s} + \sqrt{ic})} + \frac{\exp(i\sqrt{is}|x - x'|)}{2\sqrt{is}} \quad (11)$$

By making the substitution $k = \sqrt{is}$ we see this is the same propagator found using the Feynman approach [11]. We may now invert Equation 11 to obtain,

$$G(x,x',t) = -\frac{c}{2} \exp[c(|x| + |x'|) + ic^2 t] \operatorname{erfc}\left(c\sqrt{it} + \frac{|x| + |x'|}{2\sqrt{it}}\right) + \frac{1}{2\sqrt{i\pi t}} \exp\left(i \frac{(x - x')^2}{4t}\right) \quad (12)$$

Non-adiabatic Jumps

Although this example is for $c = \text{constant}$, we may use this to generate a solution for a sudden, non-adiabatic jump in the potential. This is quite simple to do. If we choose $c = -c_0$, where c_0 is a positive real number and take $\psi(x,0) = \sqrt{c_0} \exp(-c_0|x|)$ as the initial state, the system evolves with a probability density that doesn't change in time except for phase. That is because we have chosen the bound state for the attractive potential case. One way to model a sudden jump is to choose an initial state of

$\psi(x,0) = \sqrt{c_0} \exp(-c_0|x|)$, but let it evolve thereafter with $c=c'$, where $c'>0$. It can be shown that in this case [8],

$$\psi(x,t) \rightarrow \frac{2c'\sqrt{c_0}}{c_0+c'} \exp(-c'|x|) \exp(ic'^2t), t \rightarrow \infty \quad (13)$$

The total probability of it radiating away is,

$$1 - \langle |\psi(x,t)|^2 \rangle = \left(\frac{c_0 - c'}{c_0 + c'} \right)^2, t \rightarrow \infty \quad (14)$$

We see that sudden changes in potential lead to irreversible changes in the normalization of the probability density as we would expect.

Adiabatic Limit

Interestingly enough, we may also generate the adiabatic case as well using similar reasoning. The probability of it remaining in the bound state after one jump is

$$\langle |\psi(x,t)|^2 \rangle = \frac{4c_0c'}{(c_0+c')^2}, t \rightarrow \infty \quad (15)$$

Lets suppose now we break it up into two steps. We first take a small half step, let it evolve for a long time, then take a second step and let it evolve again. The result is

$$\langle |\psi(x,t)|^2 \rangle = \frac{4c_0c_1}{(c_0+c_1)^2} \frac{4c_1c_2}{(c_1+c_2)^2}, t \rightarrow \infty \quad (16)$$

Here, $c_n = c_0 + n(c' - c_0)/2$. After N such steps we have,

$$\langle |\psi(x,t,N)|^2 \rangle = 4^N \prod_{n=0}^{N-1} \frac{4c_n c_{n+1}}{(c_n + c_{n+1})^2}, t \rightarrow \infty, \quad (17)$$

where $c_n = c_0 + n(c' - c_0)/N$. The result is

$$\begin{aligned} \langle |\psi(x,t,N)|^2 \rangle = & \\ \frac{4c_0(c' + c_0(-1 + N))N}{(c' + c_0(-1 + 2N))^2} \frac{\Gamma(a_1 - 1 + N)}{\Gamma(a_1)} \frac{\Gamma(a_2 - 1 + N)}{\Gamma(a_2)} \left(\frac{\Gamma(a_3)}{\Gamma(a_3 - 1 + N)} \right)^2, & t \rightarrow \infty \end{aligned} \quad (18)$$

where

$$\begin{aligned} a_1 &= 2 + \frac{c_0}{c' - c_0} N, \\ a_2 &= 1 + \frac{c_0}{c' - c_0} N, \\ a_3 &= \frac{3}{2} + \frac{c_0}{c' - c_0} N. \end{aligned} \quad (19)$$

By taking the limit as N approaches infinity we find

$$\lim_{N \rightarrow \infty} \langle |\psi(x,t,N)|^2 \rangle = 1, t \rightarrow \infty. \quad (20)$$

This implies the probability of the particle radiating away is 0. Thus, for adiabatic changes in the potential, the normalization of the probability density is conserved, as we would infer from the Born-Fock theorem [18] on the conservation of quantum numbers.

Solution for c Linear in Time

We now consider a potential that has the following form,

$$\begin{aligned} c(t) &= -c_0, t < 0 \\ c(t) &= -c_0 - \alpha t, t > 0 \end{aligned} \quad (21)$$

Here, α is a real number. We take the bound state for $c = -c_0$ as the initial condition, which in this case is $\psi(x,0) = \sqrt{c_0} \exp(-c_0|x|)$, where α and c_0 are real constants and $c_0 > 0$. By Equation 6 and using $L[t f(t)] = -d(L[f(t)])/ds$, we find,

$$\bar{\psi}_s(0,s) - \frac{1}{\alpha} (i\sqrt{is} + c_0) \bar{\psi}(0,s) = \frac{i}{\alpha} \frac{\sqrt{c_0}}{c_0 - i\sqrt{is}} \quad (22)$$

We solve Equation 22 with the condition that the Laplace transform vanishes at $s=\infty$ and that it must also be bounded at $\pm i\infty$. The last condition is necessary for the inversion integral to exist. The solution is,

$$\begin{aligned}\bar{\psi}(0,s) &= -\frac{i\sqrt{c_0}}{\alpha} \exp\left(\frac{2}{3\alpha}(is)^{3/2} + \frac{c_0}{\alpha}s\right) \int_{-i\infty}^s ds' \frac{\exp\left(-\frac{2}{3\alpha}(is')^{3/2} - \frac{c_0}{\alpha}s'\right)}{c_0 - i\sqrt{is'}}, \alpha > 0 \\ \bar{\psi}(0,s) &= \frac{i\sqrt{c_0}}{\alpha} \exp\left(\frac{2}{3\alpha}(is)^{3/2} + \frac{c_0}{\alpha}s\right) \int_s^{\infty} ds' \frac{\exp\left(-\frac{2}{3\alpha}(is')^{3/2} - \frac{c_0}{\alpha}s'\right)}{c_0 - i\sqrt{is'}}, \alpha < 0\end{aligned}\tag{23}$$

This expression cannot be inverted in terms of elementary nor special functions. However, It can be inverted using the integral,

$$\psi(0,t) = \frac{1}{2\pi i} \int_{-i\infty+\beta}^{i\infty+\beta} ds \bar{\psi}(0,s) \exp(st)\tag{24}$$

where β is a positive constant chosen to be greater than the right most pole in the complex plane. In this case it would be chosen to be greater than 0.

One application for this would be as in the previous example where one could possibly compare adiabatic versus instantaneous change in the potential. This linear time dependence was studied in some detail by Dodonov[19] for the Coulomb potential. However, we have thus far been unable invert the Laplace transform represented by Equation 23 analytically, though numerically it is not a problem.

Solution for c Inversely Proportional to Time

Potentials that collapse in time could possibly be used to model nuclear decay. Another example might be a collapsing symmetric electric multipole in 1-D.

We choose c of the form, $c(t)=\alpha/t$, where α is a real constant. In this situation, we must be very careful. The Laplace transform of $c(t)$ doesn't exist. However, the Laplace

transform of $c(t)$ $\psi(0,t)$ does exist if we choose an initial condition that vanishes at the origin. With this restriction in mind, we proceed with the problem. We first use the identity,

$$L\left[\frac{1}{t}f(t),s\right]=\int_s^{\infty}ds' L[f(t),s'] \quad (25)$$

By Equations 25 and 6 we find

$$\bar{\psi}(0,s)=\frac{\alpha}{i\sqrt{is}}\int_s^{\infty}ds'\bar{\psi}(0,s')+\frac{1}{2\sqrt{is}}\int_{-\infty}^{\infty}dx'\exp(i\sqrt{is}|x'|)\psi(x',0) \quad (26)$$

Let,

$$u(s)=\int_s^{\infty}ds'\bar{\psi}(0,s') \quad (27)$$

Then by Equations 26 and 27 we find

$$u_s+\frac{\alpha}{i\sqrt{is}}u=-\frac{1}{2\sqrt{is}}\int_{-\infty}^{\infty}dx'\exp(i\sqrt{is}|x'|)\psi(x',0) \quad (28)$$

After solving Equation 28 we find

$$u=\int_{-\infty}^{\infty}dx'\frac{\exp(i\sqrt{is}|x'|)}{|x'|+2i\alpha}\psi(x',0) \quad (29)$$

By Equation 29 we find,

$$\bar{\psi}(0,s)=\frac{1}{2\sqrt{is}}\int_{-\infty}^{\infty}dx'\frac{|x'|\exp(i\sqrt{is}|x'|)}{|x'|+2i\alpha}\psi(x',0) \quad (30)$$

We may now invert Equation 30 to find,

$$\psi(0,t)=\frac{1}{2\sqrt{i\pi t}}\int_{-\infty}^{\infty}dx'\frac{|x'|}{|x'|+2i\alpha}\exp\left(i\frac{(x')^2}{4t}\right)\psi(x',0) \quad (31)$$

We now seek $\psi(x,t)$. To find this quantity, we first write,

$$\psi(x,t)=\int_{-\infty}^{\infty}dx'G(x,x',t)\psi(x',0) \quad (32)$$

To find G , we use the results of Equations 30, 27, 5, and 4 to find,

$$\bar{G}(x, x', s) = \frac{1}{2\sqrt{is}} \left[-\frac{2i\alpha}{|x'| + 2i\alpha} \exp(i\sqrt{is}(|x| + |x'|)) + \exp(i\sqrt{is}(|x - x'|)) \right] \quad (33)$$

We may now invert this expression to find,

$$G(x, x', t) = \frac{1}{2\sqrt{i\pi t}} \left[-\frac{2i\alpha}{|x'| + 2i\alpha} \exp\left(i \frac{(|x| + |x'|)^2}{4t}\right) + \exp\left(i \frac{(x - x')^2}{4t}\right) \right] \quad (34)$$

Solution for c with an Exponential Dependence on Time

In this case we choose $c(t) = -c_0$ for $t < 0$ and $c(t) = -c_0 + \beta \exp(-\alpha t)$ for $t > 0$, where c_0 is real such that $c_0 > 0$, β is real, and $\alpha > 0$. We choose the bound state for $c(t) = -c_0$ as the initial condition where $\psi(x, 0) = \sqrt{c_0} \exp(-c_0 |x|)$. This represents a type of impulse. One can imagine the constant attractive bound state case, where at $t=0$, the potential jumps to $-c_0 + b$, then quickly falls back to $-c_0$. This could represent a model for stimulated emission.

We use the shift formula for Laplace transforms, which is given by,

$$L[\exp(at)f(t), s] = L[f(t), s - a] \quad (35)$$

By Equations 35 and 6 we find,

$$\bar{\psi}(0, s) = \frac{\sqrt{c_0}}{s - ic_0^2} - \frac{\sqrt{i}\beta}{\sqrt{s} - \sqrt{ic_0}} \bar{\psi}(0, s + \alpha) \quad (36)$$

To obtain a solution, we could iterate this expression repeatedly to obtain the series solution,

$$\bar{\psi}(0, s) = \sum_{n=0}^{\infty} \beta^n a_n(s) \quad (37)$$

But since we already know the form of the series, we may substitute Equation 37 directly into Equation 36. After doing this and solving for the a 's by equating terms with like powers of β , we find $a_n(s)$ is given by

$$\begin{aligned} a_n(s) &= \frac{\sqrt{c_0}}{s - ic_0^2}, n = 0 \\ a_n(s) &= \frac{(-\sqrt{i})^n \sqrt{c_0}}{s + n\alpha - ic_0^2} \prod_{j=0}^{n-1} \frac{1}{\sqrt{s + j\alpha - \sqrt{i}c_0}}, n > 0 \end{aligned} \quad (38)$$

Discussion

It was shown that the time dependent Schrödinger equation with a time dependent delta function potential can be solved exactly in many special cases. We were able to show that, in contrast to the case of sudden change, the adiabatic change in the potential leads to a conservation in the normalization of the probability density of the bound state. This is a rather significant result because it proves the system is reversible to within a phase factor if the change is slow enough.

The periodic case and multi-delta function case was excluded for the sake of brevity and because they deserve a separate treatment due to the complexity of the solutions. The case of the sinusoidal time dependent potential can be treated in a similar manner as the exponential time dependent potential by representing the sine function as a sum of complex exponentials. Those two cases have also been treated elsewhere in a different context. As stated earlier the scattering problem was solved for the delta function with a strength that varied periodically in time [9] in as much as they were able to derive a transmission coefficient. We treated that same case as an initial value problem a decade before [8]. In the case of the multi-delta-function potential, this has also been recently treated in the literature [14,15] in the case of constant in time delta function potentials

and also in the case of delta function potentials moving with constant speed [13]. We also treated that case more than a decade before [8] for the case where the strength varies in time.

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